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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS	3	AUG 06	FSTA enhanced with new thesaurus edition
NEWS	4	AUG 13	CA/CAPplus enhanced with additional kind codes for granted patents
NEWS	5	AUG 20	CA/CAPplus enhanced with CAS indexing in pre-1907 records
NEWS	6	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS	7	AUG 27	USPATOLD now available on STN
NEWS	8	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
NEWS	9	SEP 07	STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS	10	SEP 13	FORIS renamed to SOFIS
NEWS	11	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	12	SEP 17	CA/CAPplus enhanced with printed CA page images from 1967-1998
NEWS	13	SEP 17	CAPplus coverage extended to include traditional medicine patents
NEWS	14	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	15	OCT 02	CA/CAPplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	16	OCT 19	BEILSTEIN updated with new compounds
NEWS	17	NOV 15	Derwent Indian patent publication number format enhanced
NEWS	18	NOV 19	WPIX enhanced with XML display format
NEWS	19	NOV 30	ICSD reloaded with enhancements
NEWS	20	DEC 04	LINPADOCDB now available on STN
NEWS	21	DEC 14	BEILSTEIN pricing structure to change
NEWS	22	DEC 17	USPATOLD added to additional database clusters
NEWS	23	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS	24	DEC 17	DGENE now includes more than 10 million sequences
NEWS	25	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS	26	DEC 17	MEDLINE and LMEMLINE updated with 2008 MeSH vocabulary
NEWS	27	DEC 17	CA/CAPplus enhanced with new custom IPC display formats
NEWS	28	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS	29	JAN 02	STN pricing information for 2008 now available
NEWS	30	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	31	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	32	JAN 28	MARPAT searching enhanced
NEWS	33	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	34	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	35	JAN 28	MEDLINE and LMEMLINE reloaded with enhancements

NEWS 36 FEB 08 STN Express, Version 8.3, now available

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 24 JANUARY 2008

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NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 09:29:09 ON 20 FEB 2008

=> file reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 09:29:37 ON 20 FEB 2008
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STRUCTURE FILE UPDATES: 19 FEB 2008 HIGHEST RN 1004621-14-0
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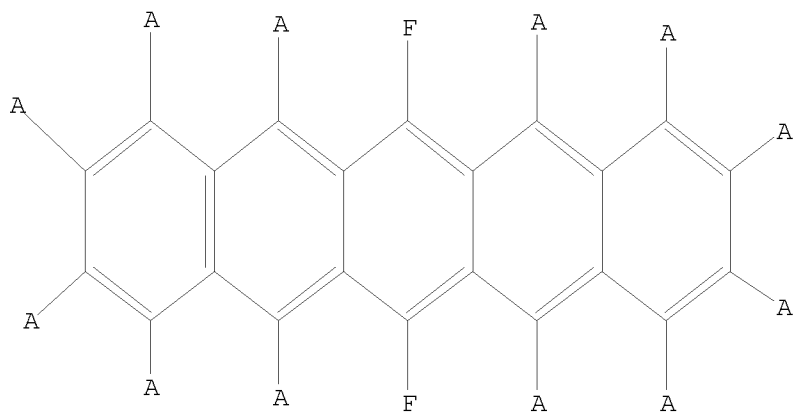
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10578259-broadest.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 09:29:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 81 TO ITERATE

100.0% PROCESSED 81 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1081 TO 2159
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

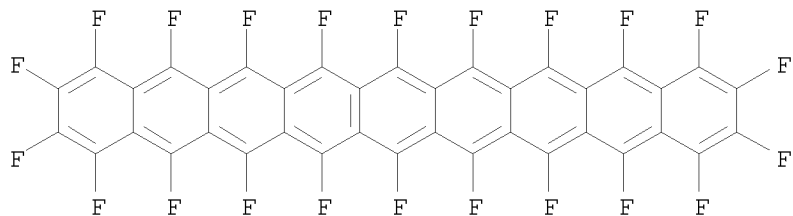
FULL SEARCH INITIATED 09:30:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1577 TO ITERATE

100.0% PROCESSED 1577 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

L3 11 SEA SSS FUL L1

=> d l3 scan

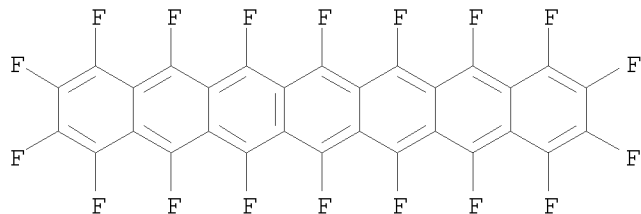
L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C38 F22



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

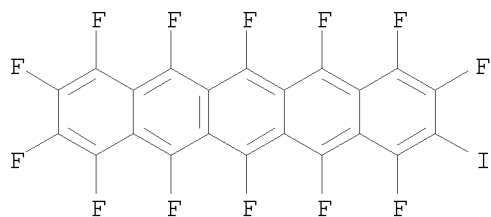
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C30 F18



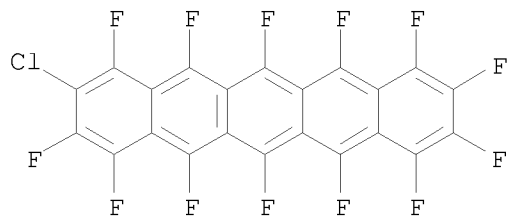
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Pentacene, 1,2,3,4,5,6,7,8,9,11,12,13,14-tridecafluoro-10-iodo-
MF C22 F13 I



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

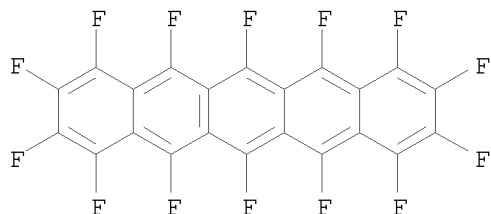
L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Pentacene, 2-chloro-1,3,4,5,6,7,8,9,10,11,12,13,14-tridecafluoro-
MF C22 Cl F13



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

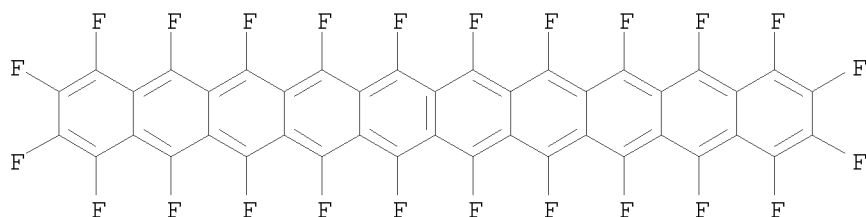
L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetrafluoro-
MF C22 F14



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 11 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C42 F24



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.82

179.03

FILE 'CAPLUS' ENTERED AT 09:30:40 ON 20 FEB 2008

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FILE LAST UPDATED: 19 Feb 2008 (20080219/ED)

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=> s 13

L4 19 L3

=> s 13 not py > 2003

19 L3

5355707 PY > 2003

L5 1 L3 NOT PY > 2003

=> s 13 not py > 2004

19 L3

4248038 PY > 2004

L6 4 L3 NOT PY > 2004

=> d 16 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 4 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:577543 CAPLUS

DOCUMENT NUMBER: 141:260225

TITLE: The essential role of H-F substitution in the
electron-phonon interactions and electron transfer in
the negatively charged acenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto
University, Sakyo-ku, Kyoto, 606-8103, Japan

SOURCE: Journal of Chemical Physics (2004), 121(5), 2356-2366
CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The single charge transfer through acenes, partially H-F substituted acenes, and fluoroacenes is discussed. The reorganization energies between the neutral mols. and the corresponding monoanions for partially H-F substituted acenes lie between those for acenes and fluoroacenes. The delocalization of the lowest unoccupied MOs (LUMO) by substituting hydrogen atoms by fluorine atoms with the highest electronegativity in every element is the main reason why the reorganization energy between the neutral mol. and the monoanion for partially H-F substituted acenes lies between those for acenes and fluoroacenes. This result implies that the neg. charged partially H-F substituted acenes would be better conductors with rapid electron transfer than the neg. charged fluoroacenes if we assume that the overlap of the LUMO between partially H-F substituted acenes is not significantly different from that between two neighboring fluoroacenes. The structures of the monoanions of acenes, fluoroacenes, and partially H-F substituted acenes are optimized under D2h geometry, and the Jahn-Teller effects in the monoanions of benzene and fluorobenzene are discussed. The vibration effect onto the charge transfer problem is also discussed. The C-C stretching modes around 1500 cm⁻¹ are the main modes converting the neutral mols. to the monoanions in acenes, fluoroacenes, and partially H-F substituted acenes. It can be confirmed from the calculational results that the C-C stretching modes around 1500 cm⁻¹ the most strongly couple to the LUMO in these mols. The main reason why the total electron-phonon coupling consts. (1LUMO) for the monoanions of acenes in which four outer hydrogen atoms are substituted by fluorine atoms are larger than those for the monoanions of acenes in which several inner hydrogen atoms are substituted by fluorine atoms is suggested. The

relationships between the electron transfer and the electron-phonon interactions are discussed. The plot of the reorganization energies against the LUMO values is found to be nearly linear. In view of these results, the relationships between the normal and superconducting states are briefly discussed.

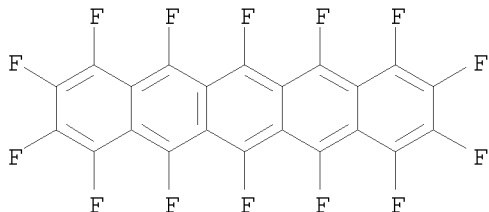
IT 646533-88-2 690975-12-3

RL: PRP (Properties)

(essential role of H-F substitution in electron-phonon interactions and electron transfer in neg. charged acenes)

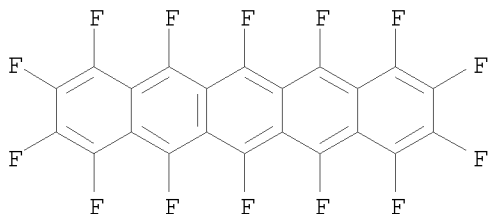
RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetrafluoro- (CA INDEX NAME)



RN 690975-12-3 CAPLUS

CN Pentacene, tetrafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:480070 CAPLUS

DOCUMENT NUMBER: 141:197895

TITLE: Perfluoropentacene: High-Performance p-n Junctions and Complementary Circuits with Pentacene

AUTHOR(S): Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Fukai, Yasushi; Inoue, Youji; Sato, Fumio; Tokito, Shizuo

CORPORATE SOURCE: Institute for Molecular Science, Okazaki, 444-8787, Japan

SOURCE: Journal of the American Chemical Society (2004), 126(26), 8138-8140

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report the synthesis and characterization of perfluoropentacene as an n-type semiconductor for organic field-effect transistors (OFETs). Perfluoropentacene is a planar and crystalline material that adopts a herringbone structure as observed for pentacene. OFETs with perfluoropentacene were constructed using top-contact geometry, and an electron mobility of 0.11 cm² V⁻¹ s⁻¹ was observed. Bipolar OFETs with

perfluoropentacene and pentacene function at both neg. and pos. gate voltages. The improved p-n junctions are probably due to the similar d-spacings of both acenes. Complementary inverter circuits were fabricated, and the transfer characteristics exhibit a sharp inversion of the output signal with a high-voltage gain.

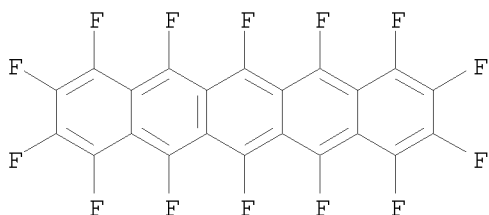
IT 646533-88-2P, Perfluoropentacene

RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)

(perfluoropentacene: high-performance p-n junctions and complementary circuits with pentacene)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:297458 CAPLUS

DOCUMENT NUMBER: 140:429323

TITLE: Inverse isotope effects and electron-phonon coupling in the positively charged deutero- and fluoroacenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8103, Japan

SOURCE: Journal of Chemical Physics (2004), 120(16), 7659-7672
CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electron-phonon interactions in the monocations of deutero- and fluoroacenes are studied and compared with those in the monocations of acenes and those in the monoanions of fluoroacenes. Because of the significant phase pattern difference between the highest occupied MOs (HOMO) and the lowest unoccupied MOs (LUMO), the frequency modes lower than 500 cm⁻¹ and the high-frequency modes around 1400 cm⁻¹ couple more strongly to the LUMO than to the HOMO, while the frequency modes around 500 cm⁻¹ and the frequency modes around 1600 cm⁻¹ couple more strongly to the HOMO than to the LUMO in fluoroacenes with D_{2h} geometry. The total electron-phonon coupling consts. for the monocations (lHOMO) are estimated and compared with those for the monoanions (lLUMO) in deutero- and fluoroacenes. The lHOMO values are estimated to be 0.418, 0.399, 0.301, 0.255, and 0.222 eV for C₆F₆ (1f), C₁₀F₈ (2f), C₁₄F₁₀ (3f), C₁₈F₁₂ (4f), and C₂₂F₁₄ (5f), resp. The lHOMO values are smaller than the lLUMO values in small fluoroacenes. But the lHOMO value decreases with an increase in mol. size less rapidly than the lLUMO value in fluoroacenes, and the lHOMO value of 0.074 eV is much larger than the lLUMO value of 0.009 eV in polyfluoroacene. The logarithmically averaged phonon frequencies for the monocations (ω_{ln},HOMO) are estimated to be larger than those for the monoanions (ω_{ln},LUMO) in fluoroacenes. This is because the C-C stretching modes around 1600 cm⁻¹ couple most strongly to the HOMO, and those around 1400 cm⁻¹ couple the most strongly to the LUMO in

fluoroacenes. The significant phase pattern difference between the HOMO and the LUMO is the main reason for the calculational results. The 1HOMO values increase much more significantly by H-F substitution than by H-D substitution in acenes. The possible inverse isotope effects in the electron-phonon interactions as a consequence of deuteration in the monocations of nanosized mols. are suggested.

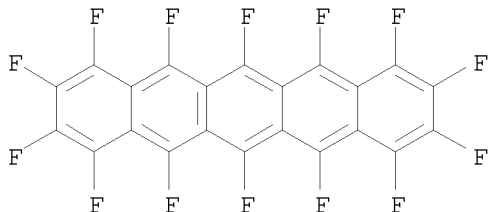
IT 690975-12-3

RL: PRP (Properties)

(inverse isotope effects and electron-phonon coupling in pos. charged deuterio- and fluoroacenes)

RN 690975-12-3 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:898555 CAPLUS

DOCUMENT NUMBER: 140:118999

TITLE: Electron-phonon interactions in the monoanions of fluoroacenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Graduate School of Engineering, Department of Material Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan

SOURCE: Journal of Chemical Physics (2003), 119(21), 11318-11328

CODEN: JCPSA6; ISSN: 0021-9606

PUBLISHER: American Institute of Physics

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Electron-phonon interactions in the monoanions of fluoroacenes such as C₆F₆ (1f), C₁₀F₈ (2f), C₁₄F₁₀ (3f), C₁₈F₁₂ (4f), and C₂₂F₁₄ (5f) are studied, and compared with those in the monoanions of acenes and deuterio-acenes. The C-C stretching modes around 1500 cm⁻¹ the most strongly couple to the lowest unoccupied MOs (LUMO) in fluoroacenes. The estimated total electron-phonon coupling consts. (1LUMO) are 0.475, 0.473, 0.350, 0.273, and 0.215 eV for 1f, 2f, 3f, 4f, and 5f, resp. The 1LUMO values for fluoroacenes are much larger than those for acenes and deuterio-acenes. Possible superconducting transition temps. (T_cs) for the monoanions of deuterio-acenes and fluoroacenes are larger than those for the monoanions of acenes. The transition temperature (T_c) value increases much more significantly by H-F substitution than by H-D substitution in acenes. The 1LUMO and T_c values significantly decrease with an increase in mol. size from the monoanions of 1f to 5f. The logarithmically averaged phonon frequencies (ω_{ln}) do not significantly change with an increase in mol. size in the monoanions of fluoroacenes. The larger displacements of C atoms in the vibronic active modes in fluoroacenes than those in deuterio-acenes due to larger atomic mass of F than that of D, and the unchanged properties of the orbital patterns of the LUMO as a consequence of H-F and H-D substitution in acenes, are the main reasons why the 1LUMO value increases much more significantly by H-F substitution than by H-D

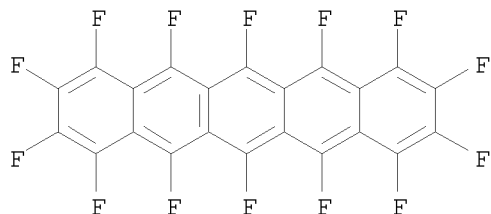
substitution, and the reason why the Tc value increases much more significantly by H-F substitution than by H-D substitution in acenes. The detailed properties of vibronic active modes and the electronic structures in the LUMO as well as the mol. wts. are closely related to the 1LUMO, ω_{ln} , and Tc values in the monoanions of fluoroacenes, deuterioacenes, and acenes.

IT 646533-88-2

RL: PRP (Properties)
(carbon-carbon bond lengths in)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)

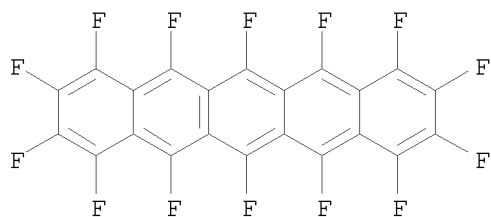


IT 645401-34-9

RL: PRP (Properties)
(electron-phonon interactions in)

RN 645401-34-9 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1-) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
38.52	217.55

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-3.20	-3.20

CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 09:46:33 ON 20 FEB 2008

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STRUCTURE FILE UPDATES: 19 FEB 2008 HIGHEST RN 1004621-14-0

DICTIONARY FILE UPDATES: 19 FEB 2008 HIGHEST RN 1004621-14-0

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

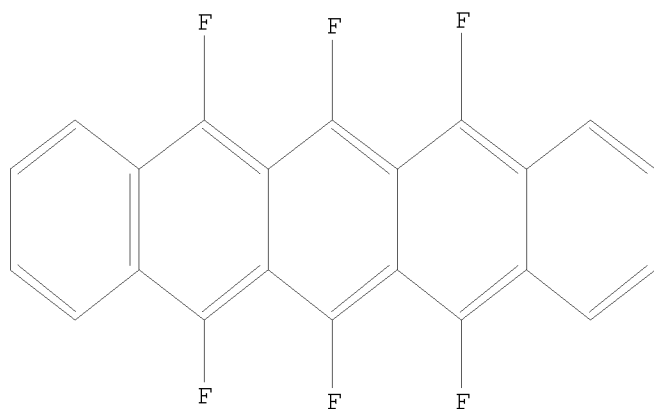
Uploading C:\Program Files\Stnexp\Queries\10578259-claim-2.str

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17

SAMPLE SEARCH INITIATED 09:46:54 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 60 TO ITERATE

100.0% PROCESSED 60 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 736 TO 1664

PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 full

FULL SEARCH INITIATED 09:46:59 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1124 TO ITERATE

100.0% PROCESSED 1124 ITERATIONS

11 ANSWERS

SEARCH TIME: 00.00.01

L9 11 SEA SSS FUL L7

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

178.36

395.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-3.20

FILE 'CAPLUS' ENTERED AT 09:47:06 ON 20 FEB 2008

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FILE LAST UPDATED: 19 Feb 2008 (20080219/ED)

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=> s 19 not 14

19 L9

L10 0 L9 NOT L4

=> s 19 not py > 2005

19 L9

3044168 PY > 2005

L11 7 L9 NOT PY > 2005

=> s 19 not py > 2004

19 L9

4248038 PY > 2004

L12 4 L9 NOT PY > 2004

=> d l12 ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 4 ANSWERS - CONTINUE? Y/(N):y

L12 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:577543 CAPLUS

DOCUMENT NUMBER: 141:260225

TITLE: The essential role of H-F substitution in the electron-phonon interactions and electron transfer in the negatively charged acenes

AUTHOR(S): Kato, Takashi; Yamabe, Tokio

CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8103, Japan

SOURCE: Journal of Chemical Physics (2004), 121(5), 2356-2366
CODEN: JCPA6; ISSN: 0021-9606
PUBLISHER: American Institute of Physics
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The single charge transfer through acenes, partially H-F substituted acenes, and fluoroacenes is discussed. The reorganization energies between the neutral mols. and the corresponding monoanions for partially H-F substituted acenes lie between those for acenes and fluoroacenes. The delocalization of the lowest unoccupied MOs (LUMO) by substituting hydrogen atoms by fluorine atoms with the highest electronegativity in every element is the main reason why the reorganization energy between the neutral mol. and the monoanion for partially H-F substituted acenes lies between those for acenes and fluoroacenes. This result implies that the neg. charged partially H-F substituted acenes would be better conductors with rapid electron transfer than the neg. charged fluoroacenes if we assume that the overlap of the LUMO between partially H-F substituted acenes is not significantly different from that between two neighboring fluoroacenes. The structures of the monoanions of acenes, fluoroacenes, and partially H-F substituted acenes are optimized under D2h geometry, and the Jahn-Teller effects in the monoanions of benzene and fluorobenzene are discussed. The vibration effect onto the charge transfer problem is also discussed. The C-C stretching modes around 1500 cm⁻¹ are the main modes converting the neutral mols. to the monoanions in acenes, fluoroacenes, and partially H-F substituted acenes. It can be confirmed from the calculational results that the C-C stretching modes around 1500 cm⁻¹ the most strongly couple to the LUMO in these mols. The main reason why the total electron-phonon coupling consts. (1LUMO) for the monoanions of acenes in which four outer hydrogen atoms are substituted by fluorine atoms are larger than those for the monoanions of acenes in which several inner hydrogen atoms are substituted by fluorine atoms is suggested. The relationships between the electron transfer and the electron-phonon interactions are discussed. The plot of the reorganization energies against the 1LUMO values is found to be nearly linear. In view of these results, the relationships between the normal and superconducting states are briefly discussed.

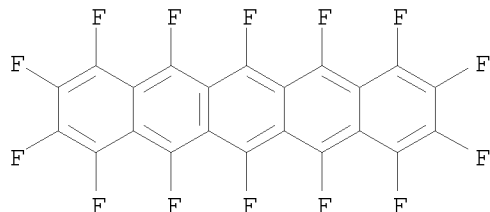
IT 646533-88-2 690975-12-3

RL: PRP (Properties)

(essential role of H-F substitution in electron-phonon interactions and electron transfer in neg. charged acenes)

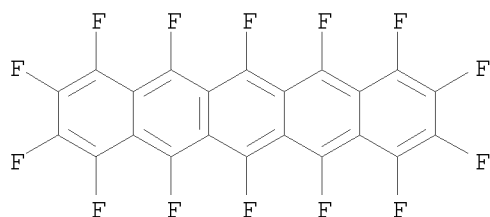
RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetrafluoro- (CA INDEX NAME)



RN 690975-12-3 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:480070 CAPLUS

DOCUMENT NUMBER: 141:197895

TITLE: Perfluoropentacene: High-Performance p-n Junctions and Complementary Circuits with Pentacene

AUTHOR(S): Sakamoto, Youichi; Suzuki, Toshiyasu; Kobayashi, Masafumi; Gao, Yuan; Fukai, Yasushi; Inoue, Youji; Sato, Fumio; Tokito, Shizuo

CORPORATE SOURCE: Institute for Molecular Science, Okazaki, 444-8787, Japan

SOURCE: Journal of the American Chemical Society (2004), 126(26), 8138-8140

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report the synthesis and characterization of perfluoropentacene as an n-type semiconductor for organic field-effect transistors (OFETs). Perfluoropentacene is a planar and crystalline material that adopts a herringbone structure as observed for pentacene. OFETs with perfluoropentacene were constructed using top-contact geometry, and an electron mobility of 0.11 cm² V⁻¹ s⁻¹ was observed. Bipolar OFETs with perfluoropentacene and pentacene function at both neg. and pos. gate voltages. The improved p-n junctions are probably due to the similar d-spacings of both acenes. Complementary inverter circuits were fabricated, and the transfer characteristics exhibit a sharp inversion of the output signal with a high-voltage gain.

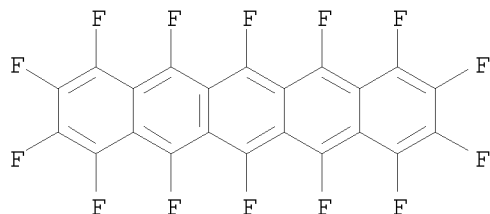
IT 646533-88-2P, Perfluoropentacene

RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)

(perfluoropentacene: high-performance p-n junctions and complementary circuits with pentacene)

RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:297458 CAPLUS
 DOCUMENT NUMBER: 140:429323
 TITLE: Inverse isotope effects and electron-phonon coupling in the positively charged deuterio- and fluoroacenes
 AUTHOR(S): Kato, Takashi; Yamabe, Tokio
 CORPORATE SOURCE: Fukui Institute for Fundamental Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8103, Japan
 SOURCE: Journal of Chemical Physics (2004), 120(16), 7659-7672
 CODEN: JCPSA6; ISSN: 0021-9606
 PUBLISHER: American Institute of Physics
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Electron-phonon interactions in the monocations of deuterio- and fluoroacenes are studied and compared with those in the monocations of acenes and those in the monoanions of fluoroacenes. Because of the significant phase pattern difference between the highest occupied MOs (HOMO) and the lowest unoccupied MOs (LUMO), the frequency modes lower than 500 cm⁻¹ and the high-frequency modes around 1400 cm⁻¹ couple more strongly to the LUMO than to the HOMO, while the frequency modes around 500 cm⁻¹ and the frequency modes around 1600 cm⁻¹ couple more strongly to the HOMO than to the LUMO in fluoroacenes with D_{2h} geometry. The total electron-phonon coupling consts. for the monocations (lHOMO) are estimated and compared with those for the monoanions (lLUMO) in deuterio- and fluoroacenes. The lHOMO values are estimated to be 0.418, 0.399, 0.301, 0.255, and 0.222 eV for C₆F₆ (1f), C₁₀F₈ (2f), C₁₄F₁₀ (3f), C₁₈F₁₂ (4f), and C₂₂F₁₄ (5f), resp. The lHOMO values are smaller than the lLUMO values in small fluoroacenes. But the lHOMO value decreases with an increase in mol. size less rapidly than the lLUMO value in fluoroacenes, and the lHOMO value of 0.074 eV is much larger than the lLUMO value of 0.009 eV in polyfluoroacene. The logarithmically averaged phonon frequencies for the monocations (ω_{ln,HOMO}) are estimated to be larger than those for the monoanions (ω_{ln,LUMO}) in fluoroacenes. This is because the C-C stretching modes around 1600 cm⁻¹ couple most strongly to the HOMO, and those around 1400 cm⁻¹ couple the most strongly to the LUMO in fluoroacenes. The significant phase pattern difference between the HOMO and the LUMO is the main reason for the calculational results. The lHOMO values increase much more significantly by H-F substitution than by H-D substitution in acenes. The possible inverse isotope effects in the electron-phonon interactions as a consequence of deuteration in the monocations of nanosized mols. are suggested.

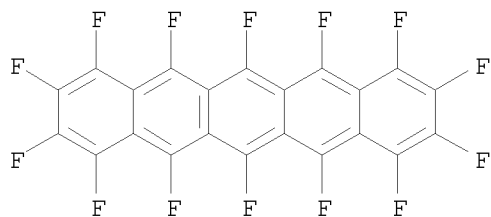
IT 690975-12-3

RL: PRP (Properties)

(inverse isotope effects and electron-phonon coupling in pos. charged deuterio- and fluoroacenes)

RN 690975-12-3 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1+) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

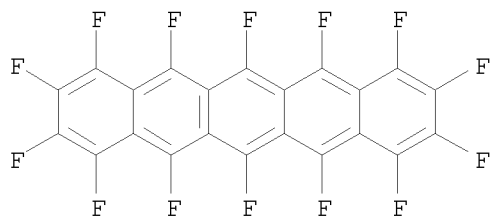
ACCESSION NUMBER: 2003:898555 CAPLUS
 DOCUMENT NUMBER: 140:118999
 TITLE: Electron-phonon interactions in the monoanions of fluoroacenes
 AUTHOR(S): Kato, Takashi; Yamabe, Tokio
 CORPORATE SOURCE: Graduate School of Engineering, Department of Material Chemistry, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan
 SOURCE: Journal of Chemical Physics (2003), 119(21), 11318-11328
 CODEN: JCPSA6; ISSN: 0021-9606
 PUBLISHER: American Institute of Physics
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Electron-phonon interactions in the monoanions of fluoroacenes such as C₆F₆ (1f), C₁₀F₈ (2f), C₁₄F₁₀ (3f), C₁₈F₁₂ (4f), and C₂₂F₁₄ (5f) are studied, and compared with those in the monoanions of acenes and deutero-acenes. The C-C stretching modes around 1500 cm⁻¹ the most strongly couple to the lowest unoccupied MOs (LUMO) in fluoroacenes. The estimated total electron-phonon coupling consts. (λLUMO) are 0.475, 0.473, 0.350, 0.273, and 0.215 eV for 1f, 2f, 3f, 4f, and 5f, resp. The λLUMO values for fluoroacenes are much larger than those for acenes and deutero-acenes. Possible superconducting transition temps. (T_cs) for the monoanions of deutero-acenes and fluoroacenes are larger than those for the monoanions of acenes. The transition temperature (T_c) value increases much more significantly by H-F substitution than by H-D substitution in acenes. The λLUMO and T_c values significantly decrease with an increase in mol. size from the monoanions of 1f to 5f. The logarithmically averaged phonon frequencies (ω_{ln}) do not significantly change with an increase in mol. size in the monoanions of fluoroacenes. The larger displacements of C atoms in the vibronic active modes in fluoroacenes than those in deutero-acenes due to larger atomic mass of F than that of D, and the unchanged properties of the orbital patterns of the LUMO as a consequence of H-F and H-D substitution in acenes, are the main reasons why the λLUMO value increases much more significantly by H-F substitution than by H-D substitution, and the reason why the T_c value increases much more significantly by H-F substitution than by H-D substitution in acenes. The detailed properties of vibronic active modes and the electronic structures in the LUMO as well as the mol. wts. are closely related to the λLUMO, ω_{ln}, and T_c values in the monoanions of fluoroacenes, deuteroacenes, and acenes.

IT 646533-88-2
 RL: PRP (Properties)
 (carbon-carbon bond lengths in)

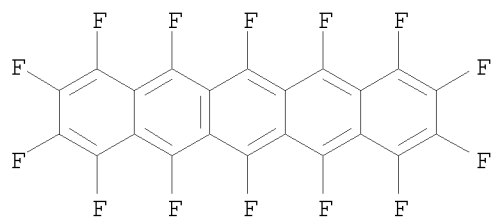
RN 646533-88-2 CAPLUS

CN Pentacene, 1,2,3,4,5,6,7,8,9,10,11,12,13,14-tetradecafluoro- (CA INDEX NAME)



IT 645401-34-9
 RL: PRP (Properties)
 (electron-phonon interactions in)
 RN 645401-34-9 CAPLUS

CN Pentacene, tetradecafluoro-, radical ion(1-) (9CI) (CA INDEX NAME)



REFERENCE COUNT:

90

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